Reactive Transport Modeling of CO_2 Emissions and Calcite Precipitation Kinetics in Dryland Agriculture

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More than 40% of the Earth's land cover has been designated as drylands and deserts (Reynolds et al 2007). Growing populations require that drylands be used for agriculture, while providing a home to more than 38% of the world's population (Reynolds et al. 2007; MEA 2005). Dryland agriculture is unsustainable because of the vast amount of water used in a water-limited environment. Additionally, these waters have high salinity, regional evapotranspiration exceeds precipitation and drainage is poor, leading to salt accumulation in soils.

Calcite has low solubility and oversaturation in irrigation waters leads to calcite precipitation after extensive evapotranspiration (Szykiewicz et al 2015):

$2HCO_3^-{}_{(aq)} + Ca^{2+}{}_{(aq)} \leftrightarrow CaCO_{3(s)} + CO_{2(g)} + H_2O_{(l)}$

Field work has identified the precipitation of the secondary pedogenic calcite and quantified the production of CO_2, highlighting an unforseen pathway that might impact carbon allocations and climate.

Reactive transport modeling is a powerful tool that can be used to understand physical, hydrological, and kinetic controls on dynamic systems where soil-gas-water-vegetation interactions drive complex precipitation kinetics and solute/gas transport. Simulations of field and column experiments involving CO_2 transport and calcite kinetics were performed using the parallel non-isothermal multiphase reactive transport program TOUGHREACT.

Preliminary simulations have successfully captured gas and phase CO_2 diffusive and advective transport coupled to air-water exchange during infiltration and capillary retention in a flow-through column experiment. Work is currently aimed at analyzing the impact of pressure pumping and diurnal temperature changes on calcite dissolution and precipitation in the column experiment. Furthermore, the modeling of biotic controls on soil respiration, such as root respiration, will help delineate the contribution that biotic and abiotic processes have on carbon dioxide efflux.

Reference: Reynolds, J. F. et al (2007) Science, 316, 847–851;Millennium Ecosystem Assessment, (2005).Press, Washington, DC.; Szynkiewicz A., et al. (2015) Chemical Geology 411, 336.